

ABSTRACT

A process is provided for the high throughput screening of binding of ligands to macromolecules using high resolution powder diffraction data including producing a first sample slurry of a selected polycrystalline macromolecule material and a solvent,

5 producing a second sample slurry of a selected polycrystalline macromolecule material, one or more ligands and the solvent, obtaining a high resolution powder diffraction pattern on each of said first sample slurry and the second sample slurry, and, comparing the high resolution powder diffraction pattern of the first sample slurry and the high resolution powder diffraction pattern of the second sample slurry whereby a difference in the high

10 resolution powder diffraction patterns of the first sample slurry and the second sample slurry provides a positive indication for the formation of a complex between the selected polycrystalline macromolecule material and at least one of the one or more ligands.

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